

University of Southern Denmark

3rd Workshop on Model Reduction of Complex Dynamical Systems - MODRED 2017 -

Department of Mathematics and Computer Science (IMADA)

January 11–13, 2017





Welcome

Dear Colleagues,

welcome to the

3rd Workshop on Model Reduction of Complex Dynamical Systems.

The workshop program features 5 keynote lectures and 39 contributed talks. Our special thanks go to the keynote speakers for accepting our invitation. We thank all the contributors for their talks.

Moreover, we express our gratitude towards Diana Noatsch-Liebke and Janine Holzmann at MPI Magdeburg and Lone Seidler-Petterson at SDU for their administrative support and Nicky Cordua Mattsson and Christian Valdemar Hansen for their local assistance.

We gratefully acknowledge support of the European Union Model Reduction Network (EU-MORNET) and of IMADA/SDU.

We are looking forward to exciting talks, fruitful discussions and inspiring encounters.

Scientific Committee

Peter Benner, MPI Magdeburg Heike Faßbender, TU Braunschweig Michael Hinze, University of Hamburg Tatjana Stykel, University of Augsburg Ralf Zimmermann, SDU Odense

Organizational issues

On-site registration: from Wednesday, January 11, 8:00 a.m. **Opening:** Wednesday, January 11, 8:50 a.m. **Closing:** Friday, January 13, 12:00 p.m.

Scientific Topics: Computational methods for model order reduction of dynamical systems, in particular (but not limited to)

- system-theoretic methods (e.g., system balancing, Hankel norm approximation)
- rational interpolation (moment-matching, H2-optimal reduction, ...)
- POD and generalizations
- reduced basis methods
- tensor-based techniques (PGD, low-tensor-rank approximations, ...)
- data-driven methods, e.g., vector fitting and Loewner matrix and pencil based approaches
- surrogate modeling for design and optimization

The range of applications includes network systems, computational electromagnetics, computational nanoelectronics, structural mechanics, fluid dynamics, control of PDEs and data assimilation.

Travel and local information

If you arrive by plane it is easiest to travel to Copenhagen Airport. From Copenhagen Airport you take the train to Copenhagen Central Station. At Copenhagen Central Station you take the train to Odense Central Station (Odense St). You can buy the train ticket to Odense at the Airport. Please remember to buy a separate seat ticket to make sure to be seated the whole journey. There are train connections every 30min during daytime from Copenhagen Airport to Odense St.

It is recommended to travel to Odense by train if you come from northern Germany or Southern Sweden. You can use the site "Rejseplanen"

http://www.rejseplanen.dk/

to plan your journey in Denmark.

The conference hotels are all in walking distance of Odense St, see Fig. 1.



Figure 1: Location of the hotels 'Windsor', 'Ansgar', 'Plaza' and 'City Hotel Odense' in relation to the train station (Odense St).

From Odense St, bus lines 41, 42 or 44 will take you to SDU campus (almost every 10min, direction: Syddanske Universitetet). If you are lodging at City Hotel Odense, get on at bus stop 'Hans Mules Gade' right in front of the hotel. Bus rides are 23DKK and require cash.

An interactive campus map is available at:

https://clients.mapsindoors.com/sdu/573f26e4bc1f571b08094312

Conference Dinner: The conference dinner takes place on January 12, 2017 at 7:00 pm at "Den Gamle Kro" (the old inn), which is located in the city center in walking distance to the conference hotels. The dinner is included in the conference fees. (http://www.dengamlekro.eu/)

@Internet access

On campus, EDUROAM is available. You have also free access to the 'SDU-GUEST' network, which is not password protected.

Funding

This workshop is supported by IMADA and by the European Model Reduction Network (EU-MORNET).

The EU-MORNET aims at bringing together all major groups in Europe working on a range of model reduction strategies with applications in many domains of science and technology. The increasing complexity of mathematical models used to predict real-world systems, such as climate or the human cardiovascular system, has led to a need for model reduction, which means developing systematic algorithms for replacing complex models with far simpler ones, that still accurately capture the most important aspects of the phenomena being modeled. The Action will emphasize model reduction topics in several themes:

- 1. design, optimization, and control theory in real-time with applications in engineering;
- 2. data assimilation, geometry registration, and parameter estimation with a special attention to real-time computing in biomedical engineering and computational physics;
- 3. real-time visualization of physics-based simulations in computer science;
- 4. the treatment of high-dimensional problems in state space, physical space, or parameter space;
- 5. the interactions between different model reduction and dimensionality reduction approaches;

The focus of the Action is methodological; however, a wide range of both scientific and industrial problems of high complexity is anticipated to motivate, stimulate, and ultimately demonstrate the meaningfulness and efficiency of the Action. The main objective of the Action is to significantly bringing down computation times for realistic simulations and cosimulations of industrial, scientific, economic and societal models by developing appropriate model reduction methods.

For more information and participation, visit http://www.eu-mor.net/.

SDU and IMADA

Odense university was founded in 1966. The University of Southern Denmark was established in 1998 through a merger involving Odense University, the Southern Denmark School of Business and Engineering and South Jutland University Centre.

The Department of Mathematics and Computer Science was founded in 1972. The Department is commonly known by its Danish acronym IMADA.

IMADAs research covers a broad area, is interdisciplinary and includes both pure and applied research. The departments geometry group is part of a pioneering collaboration with particle physicists. A new area of focus at IMADA is numerical mathematical modeling, where the goal is to use mathematical modeling and simulation to provide scientific understanding. Based on IMADAs research on efficient algorithms, a platform has been established for optimization in industry involving collaboration with public and private companies. IMADAs research within algorithms contributes to the development of quality measures for online algorithms as well as to the unveiling of evolutionary relationships between groups of organisms. The department also houses the Center for Science and Mathematics Education, which together with regional partners develops courses and degree programmes for school teachers.

IMADA offers a wide range of degree programmes in mathematics, computer science and didactics:

- Bachelor's and Master's degrees in applied mathematics, computer science, mathematics and mathematics and economics
- Masters degree in science education

Schedule

11
January
Wednesday,
2017:
MODRED 2017

	A.T. Patera: Parametrized model order reduction for component-to-system synthesis Coffee break	
	ee break	mponent-to-system synthesis Room: U1
	,	
	Room: U1	Room: U26
	F. Naets: A-priori element selection and weighting for	A. Castagnotto: Interpolatory methods for H_{∞} model
	hyper-reduction in nonlinear structural dynamics	reduction of MIMO systems
	M. Salewski: Symmetry reduction without equivariance	P. Goyal: Interpolation-based optimal model reduc-
	in reduced order models	tion for a class of descriptor systems with application to
		Navier-Stokes equations
11:30-12:00 C.	C. Kweyu: Reduced basis method for Poisson-	M. Hund: Parametrized Sylvester equations in model
Boltz	Boltzmann equation	order reduction
12:00–13:30 Lune	Lunch break	
13:30–14:30 S. G	S. Görtz: Reduced order models for aerodynamic applications, loads and MDO	ations, loads and MDO Room: U1
Rooi	Room: U1	Room: U26
14.30-15.00 S K	S. Klus: Dynamic mode decomposition and extensions	N. Banagaaya: Snarse MOB for large-scale models with
	and a limit in the account and a contract and a	
		many inputs
10:00-10:30 A. S	A. Sauerbrei: An adaptive sampling strategy for MIMO	M. Billaud-Friess: A dynamical model order reduc-
SULTO	surrogate models based on merging (Co-)kriging and	tion method for the solution of parameter-dependent
POD		dynamical systems
15:30–16:00 Coffe	Coffee break	
Rooi	Room: U1	Room: U26
16:00–16:30 P. G	P. Gelß: SLIM-Decomposition of tensor train operators	J. Fehr: ISTEP as an example of nonlinear non-intrusive
for n	for nearest-neighbor interaction networks	model order reduction technique
16:30–17:00 F. N	F. Nüske: Variational tensor approach to the rare-event	Y. Yue: Parametric model order reduction for efficient
kinet	kinetics of macromolecular systems	uncertainty quantification in the electro-thermal analysis
$17.00-17.30$ T \mathbf{x}	T von Larchan. Annlieation of a tansor moduet do	
	composition method to turbulent data	
-		

12
January
Thursday,
2017:
MODRED 2017

$10:00{-}10:30$		
	Cottee break	
	Room: U1	Room: U70
$10{:}30{-}11{:}00$	Y. Lu: Interpolation strategy for parametric QBMOR	M. Opmeer: Decay of singular values for infinite-dimen-
	for gas pipeline-networks	sional control systems
$11:00{-}11:30$	P. Mlinarić: Model reduction of network systems by	C. Bertram: Randomized balanced POD for conti-
	clustering	nuous-time MIMO LTI systems
11:30-12:00	B. Liljegren-Sailer: On structure preserving model	S. Werner: Hankel-norm approximation of descriptor
	order reduction for damped wave propagation on	systems
	networks	
$12:00{-}14:00$	Lunch break	
14:00-14:30	J. Saak: Replicability, Reproducibility and Reusability for Model Order Reduction (RRR4MOR)	r Model Order Reduction (RRR4MOR) Room: U1
	Room: U1	Room: U7
$14:30{-}15:00$	C. Gräßle: POD reduced order modeling for evolution	P. Kürschner: Time- and frequency-limited balanced
	equations utilizing arbitrary finite element discretizations	truncation for large-scale systems
$15:00{-}15:30$	E. Gildin: Online adaptive local-global POD-DEIM	I.V. Gosea: Balanced truncation for linear switched sys-
	model reduction for fast simulation of flows in hetero-	tems
	geneous media	
$15:30{-}16:00$	Coffee break	
	Room: U1	Room: U7
$16:00{-}16:30$	J. Heiland: Space-time Galerkin POD for optimal	A. Benaceur: Improving the computational efficiency
	control of Burgers' equation	of a reduced order model for time-dependent non-linear
		PDEs
$16:30{-}17:00$	R. O'Connor: Reduced basis methods for the design of	V. Bykov: Singularly perturbed vector fields, model
	stabilizing feedback controllers	reduction of reacting flow systems
$17{:}00{-}17{:}30$	J. Bremer: Towards fast optimal control of CO ₂ metha-	X. Cheng: Model reduction of second-order electrome-
	nation reactors via POD-DEIM	chanical swing equations with structural preservation
10.00	Confournas Disson	
13:00	Conterence Dinner	

$9:00{-}10:00$	09:00–10:00 H. Sandberg: Structured model reduction of networks of passive systems	f passive systems Room: U1
0:00-10:30	10:00–10:30 Coffee break	
	Room: U1	Room: U26
0:30-11:00	10:30–11:00 C. Himpe: Towards empirical-Gramian-based model L. Zhou: A novel POD-based model order reduction at	L. Zhou: A novel POD-based model order reduction at
	reduction for nonlinear DAEs	the substructure level for nonlinear structural analysis
1:00-11:30	11:00–11:30 M. Cruz Varona: Krylov subspace methods for model Z. Tomljanović: Damping optimization of parameter	Z. Tomljanović: Damping optimization of parameter
	reduction of MIMO quadratic-bilinear systems	dependent mechanical systems by rational interpolation
1:30-12:00	11:30–12:00 D. Khlopov: Automatic model reduction of differential	S. van Ophem: Parametrized model order reduction
	algebraic systems by proper orthogonal decomposition	for second order systems with a low rank change in the
		system matrices
12:00–12:10 Closing	Closing	Room: U1
12:10	Lunch	

MODRED 2017: Friday, January 13

Contents

Welcome	i
Organizational issues	ii
Travel and local information	ii
@Internet access	v
Funding	v
SDU and IMADA	v
Schedule vi	ii
Keynotes	1
	2
Data-driven MOR methods for efficient simulation of infrastructure networks (Sara Grundel)	3
Parametrized model order reduction for component-to-system synthesis (Anthony	4 5
	$\frac{5}{6}$
Contributed talks	7
Sparse MOR for large-scale models with many inputs (<i>Nicodemus Banagaaya</i> , Lihong Feng, Peter Benner)	8
Improving the computational efficiency of a reduced order model for time-dependent	-
non-linear PDEs (Amina Benaceur, Virginie Ehrlacher, Alexandre Ern)	9
Randomized balanced POD for continuous-time MIMO LTI systems (<i>Christian</i> Bertram, Heike Faßbender) 1	0
A dynamical model order reduction method for the solution of parameter-dependent	
dynamical systems (Marie Billaud-Friess)	1
Towards fast optimal control of CO_2 methanation reactors via POD-DEIM (<i>Jens</i>	
Bremer, Pawan Goyal, Lihong Feng, Peter Benner, Kai Sundmacher) 1	2
Singularly perturbed vector fields, model reduction of reacting flow systems (<i>Vi-atcheslav Bykov</i>) 1	3

Interpolatory methods for H_{∞} model reduction of MIMO systems (<i>Alessandro</i> Castagnotto)	14
Model reduction of second-order electromechanical swing equations with struc-	1.
tural preservation (Xiaodong Cheng)	15
Krylov subspace methods for model reduction of MIMO quadratic-bilinear sys- tems (Maria Cruz Varona, Elcio Fiordelisio Junior, Boris Lohmann)	16
ISTEP as an example of nonlinear non-intrusive model order reduction technique (Dennis Grunert, Jörg Fehr)	17
SLIM-Decomposition of tensor train operators for nearest-neighbor interaction networks $(Patrick \ Gel\beta)$	18
Online adaptive local-global POD-DEIM model reduction for fast simulation of	10
flows in heterogeneous media (Eduardo Gildin, Yalchin Efendiev, Victor	19
Calo, Yanfang Yang)	15
C. Antoulas)	20
Interpolation-based optimal model reduction for a class of descriptor systems with	
application to Navier-Stokes equations (<i>Peter Benner, Pawan Goyal</i>)	21
POD reduced order modeling for evolution equations utilizing arbitrary finite	
element discretizations (Carmen Gräßle, Michael Hinze)	22
Space-time Galerkin POD for optimal control of Burgers' equation (Manuel Bau-	26
mann, Peter Benner, Jan Heiland)	23
Towards empirical-Gramian-based model reduction for nonlinear DAEs (<i>Peter</i> Benner, Sara Grundel, Christian Himpe)	24
Parametrized Sylvester equations in model order reduction (Manuela Hund, Jens Saak)	25
Automatic model reduction of differential algebraic systems by proper orthogo- nal decomposition (<i>Dmytro Khlopov, Michael Mangold, Lihong Feng, Peter</i> <i>Benner</i>)	26
Dynamic mode decomposition and extensions (<i>Stefan Klus</i>)	27
Reduced basis method for Poisson-Boltzmann equation (<i>Cleophas Kweyu, Lihong</i>	21
Feng, Matthias Stein, Peter Benner)	28
Time- and frequency-limited balanced truncation for large-scale systems ($Patrick$	
Kürschner)	29
Application of a tensor product decomposition method to turbulent data (<i>Thomas</i> von Larcher, Rupert Klein, Reinhold Schneider, Sebastian Wolf, Benjamin	
Huber)	30
On structure preserving model order reduction for damped wave propagation on networks (<i>Björn Liljegren-Sailer</i> , <i>Herbert Egger</i> , <i>Thomas Kugler</i> , <i>Nicole</i> <i>Marheineke</i>)	31
Interpolation strategy for parametric QBMOR for gas pipeline-networks (<i>Yi Lu</i> ,	01
Nicole Marheineke, Jan Mohring)	32
Model reduction of network systems by clustering (<i>Peter Benner, Sara Grundel,</i> <i>Peter Mlinaric</i>)	33

A-priori element selection and weighting for hyper-reduction in nonlinear struc-	
tural dynamics $(Frank Naets)$	34
Variational tensor approach to the rare-event kinetics of macromolecular systems	
$(Feliks N \ddot{u} s k e) \dots $	35
Reduced basis methods for the design of stabilizing feedback controllers (<i>Robert</i>	
O'Connor, Martin Grepl)	36
Parametrized model order reduction for second order systems with a low rank	
change in the system matrices (Sjoerd van Ophem, Elke Deckers, Wim	
Desmet)	37
Decay of singular values for infinite-dimensional control systems (Mark Opmeer)	38
Replicability, Reproducibility and Reusability for Model Order Reduction (RRR	
4 MOR (Jens Saak)	39
Symmetry reduction without equivariance in reduced order models (Matthew	
Salewski)	40
An adaptive sampling strategy for MIMO surrogate models based on merging	
(Co-)kriging and POD (Anna Sauerbrei, Ralf Zimmermann)	41
Damping optimization of parameter dependent mechanical systems by rational	
interpolation (Zoran Tomljanovic, Christopher Beattie, Serkan Gugercin) .	42
Hankel-norm approximation of descriptor systems (Steffen Werner, Peter Benner)	43
Parametric model order reduction for efficient uncertainty quantification in the	
electro-thermal analysis of nanoelectronic devices (Yao Yue, Lihong Feng,	
Peter Meuris, Wim Schoenmaker, Peter Benner)	44
A novel POD-based model order reduction at the substructure level for nonlinear	
structural analysis (Lei Zhou, Jaan-Willem Simon, Stefanie Reese)	45

Author Index

47

Keynotes

In alphabetical order by *presenting author*. If there are several authors, the invited author is indicated by an asterisk^{*}.

Reduced order models for aerodynamic applications, loads and MDO

Stefan Görtz^{*}, Matteo Ripepi, Thomas Franz, Mohammad Abu-Zurayk German Aeropace Center (DLR), Institute of Aerodynamics and Flow Technology, Braunschweig, Germany

Reduced Order Models (ROMs) have found widespread application in fluid dynamics and aerodynamics. In their direct application to Computational Fluid Dynamics (CFD) ROMs seek to reduce the computational complexity of a problem by reducing the number of degrees of freedom rather than simplifying the physical model. Here, parametric nonlinear ROMs based on high-fidelity CFD are used to provide approximate flow solutions, but at lower evaluation time and storage than the original CFD model. ROMs for both steady and unsteady aerodynamic applications are presented. We consider ROMs combining proper orthogonal decomposition (POD) and Isomap, which is a manifold learning method, with interpolation methods as well as physics-based ROMs, where an approximate solution is found in the POD-subspace by minimizing the corresponding steady or unsteady flow-solver residual. In terms of the nonlinear unsteady least-squares ROM algorithm, we present the details of an improved accelerated greedy missing point estimation procedure which is used in the offline phase to select a subset of the unsteady residual for reasons of computational efficiency during the online prediction phase. The issue of how to best train the ROM with high-fidelity CFD data is also addressed. The goal is to train ROMs that yield a large domain of validity across all parameters and flow conditions at the expense of a relatively small number of CFD solutions.

The different ROM methods are demonstrated on a wide-body transport aircraft configuration at transonic flow conditions. The steady ROMs are used to predict the static aeroelastic loads in the context of multidisciplinary optimization (MDO), where a structural model is to be sized for the (aerodynamic) loads. They are also used in a process where an a priori identification of the most critical static load cases is of interest and the sheer number of load cases to be considered does not lend itself to high-fidelity CFD. The unsteady nonlinear least-squares ROM approach is applied to modeling discrete gusts of different amplitude and length in the context of rapid evaluation of gust-induced air loads.

Data-driven MOR methods for efficient simulation of infrastructure networks

Sara Grundel

Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg

Our research is embedded into the goal to reform the energy landscape by using green technology. Sustainable energy sources tend to be decentralized and uncertain; for example, we cannot predict with much precision the occurrence of wind and sunshine. Therefore, uncertainty quantification and truly transient simulation are necessary to understand the behavior of these energy generation and transportation systems. In the management of these systems, multiple time simulations are desired to support decision making. Increasing the efficiency of the simulations is therefore crucial.

The challenge is to combine complex systems as well as large quantities of data. In efficient modelling and simulation of infrastructure networks we deal with hierarchical system, where the outer structure is typically the network. In the fields of big data and efficient large-scale simulations, a great deal of research is currently being conducted. We show what methods can be used for our problems. We discuss how to deal with the hyperbolic nature that arises for example in gas and water network or the difficulties that arise from Differential Algebraic Equations, which is one typical way to discribe the full system. We talk about what we can learn from the linearized system and when it could be useful to use a simplification like that, but also talk about efficient methods to simulate the full nonlinear system.

Model order reduction in pattern formation

Bülent Karasözen

Middle East Technical University, Ankara, Turkey

The prediction and estimation of spatio-temporal patterns in non-equilibrium complex systems occurring in biology, chemistry and physics is an active research field. The pattern occur in reaction diffusion systems in form of Turing pattern as a results of diffusion driven instability or in cross-diffusion systems resulting by a gradient in the concentration of one species inducing a flux of another species. The computation of the steady state solutions in pattern formation takes a very long time. In this talk we compare two reduced order modelling methods proper orthogonal decomposition (POD) and dynamic mode decomposition (DMD) for the Allen-Cahn, Fitzhugh-Nagumo, complex Ginzburg Landau equation and inhomogeneous Brusselator with cross-diffusion. We show that the reduced order solutions have high accuracy with large speed-up factors compared with the full order solutions resulting from discontinuous Galerkin finite element discretization in space and backward Euler in time.

Parametrized model order reduction for component-to-system synthesis

Anthony T. Patera

Massachusetts Institute of Technology, Cambridge, MA

In this talk we describe and demonstrate a model order reduction methodology for efficient treatment of large engineering systems with many (spatially distributed) parameters. The approach is relevant in many-query, real-time, and interactive contexts such as design, shape and topology optimization, parameter estimation, monitoring and classification, reconditioning, and education.

The numerical approach comprises four principal ingredients: component-to-system synthesis, formulated as a static-condensation procedure; parametrized model order reduction, informed by (i) evanescence arguments at component interfaces (port reduction, effected by a transfer eigenproblem), and (ii) low-dimensional parametric manifolds in component interiors (bubble reduction, effected by reduced basis techniques); offline-online computational decomposition strategies; and parallel calculation, implemented in a cloud environment. We provide examples in acoustics, linear elasticity, and also nonlinear elasticity.

Structured model reduction of networks of passive systems

Henrik Sandberg

KTH Royal Institute of Technology, Stockholm

Large-scale networks of interconnected dynamical systems appear abundantly in the natural and engineering sciences and examples range from chemical reaction networks to the electrical power grid and intelligent transportation systems. In this presentation, the model reduction problem for such complex networked systems will be discussed. In particular, reduction is performed by clustering subsystems that show similar behavior and subsequently aggregating their states, leading to a reduced-order networked system that allows for an insightful interpretation. The clusters are chosen on the basis of controllability and observability analysis of associated edge systems, leading to a reduction procedure that preserves synchronization properties and allows for the derivation of an a priori error bound.

This is joint work with Bart Besselink at the University of Groningen.

Contributed talks

In alphabetical order by *presenting author*. If there are several authors, the presenting author is indicated by an asterisk * .

Sparse MOR for large-scale models with many inputs

Nicodemus Banagaaya^{*}, Lihong Feng, Peter Benner Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg

Simulation of very large-scale models with millions of state variables and hundreds or even thousands of inputs and outputs is very difficult to be done in acceptable time. Model order reduction (MOR) aims to reduce the computational burden by generating reduced-order models (ROMs) that are faster and cheaper to be simulated, yet accurately represent the behavior of the original large-scale system. However, models with numerous inputs and outputs are challenging for MOR, and most existing MOR methods produce large and dense ROMs for such systems. Recently, the block-diagonal structured MOR method for electrothermal coupled problems with many inputs (BDSM-ET) was proposed. The BDSM-ET method leads to sparser reduced-order models (ROMs) compared to the existing MOR methods. Simulation of a very large-scale model with up to one million of state variables shows that the BDSM-ET method achieves significant speed-up as compared with the existing MOR methods.

Improving the computational efficiency of a reduced order model for time-dependent non-linear PDEs

Amina Benaceur^{1,2,*}, Virginie Ehrlacher¹, Alexandre Ern¹ ¹University Paris-Est, CERMICS (ENPC), France, ²EDF R&D, France

We address the reduced order modeling of parameterized transient non-linear and nonaffine partial differential equations (PDEs) as in Daversin and Prud'homme (2015). In practice, both the treatment of non-affine terms and non-linearities result in an empirical interpolation method (EIM) that may not be affordable although it is performed 'offline', since it requires to compute various non-linear trajectories using the full order model. An alternative to the EIM has been recently proposed in Daversin and Prud'homme (2015) so as to alleviate its cost by enriching progressively the EIM using the computed reduced basis functions.

In the present work, we adapt the ideas of Grepl et al. (2007) to transient PDEs so as to propose an algorithm that solely requires as many full-model computations as the number of functions that span both the reduced basis and the EIM spaces. The computational cost of the procedure can therefore be substantially reduced compared to the standard strategy. Finally, we discuss possible variants of the present approach.

Randomized balanced POD for continuous-time MIMO LTI systems

Christian Bertram^{*}, Heike Faßbender

Technische Universität Braunschweig, Institut Computational Mathematics, AG Numerik

In [1] Yu and Chakravorty presented an algorithm for the reduction of discrete-time LTI systems with many inputs and outputs. They proposed a BPOD-like method but used random inputs to excite all inputs at the same time to generate only one trajectory. We will present an extension of this algorithm to handle the continuous-time case. A reasonable discretization has to be found to cover the correct frequency range. Furthermore, a method to enhance accuracy in both, the discrete- and continuous-time algorithm, is presented.

[1] D. Yu, S. Chakravorty. A Computationally Optimal Randomized Proper Orthogonal Decomposition Technique. arXiv, 1509.05705v3.

A dynamical model order reduction method for the solution of parameter-dependent dynamical systems

Marie Billaud-Friess

Ecole Centrale de Nantes, Département Informatique et Mathématiques

This talk is concerned with model order reduction for solving parameter-dependent non linear dynamical systems. A projection-based method onto a time-dependent low-dimensional reduced space is proposed so that it can be interpreted as a dynamical low-rank approximation method but with a subspace point of view with a uniform control of the error over the parameter set. Then, it is closer to a Reduced Basis method with time-dependent reduced basis. The reduced approximation is obtained by Galerkin projection leading to a reduced dynamical system with a modified flux which takes into account the time dependency of the reduced spaces. An efficient a posteriori error estimate is derived and used for the greedy construction of the time dependent reduced spaces. The applicability of our method is illustrated through several numerical experiments on both linear and non-linear test cases.

Towards fast optimal control of CO_2 methanation reactors via POD-DEIM

Jens Bremer^{*,1}, Pawan Goyal¹, Lihong Feng¹, Peter Benner^{1,2}, Kai Sundmacher^{1,2} ¹Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg ²Otto-von-Guericke University, Magdeburg

Utilizing volatile renewable energy sources (e.g., solar, wind) for chemical production systems requires a deep understanding of their dynamic operation modes. Taking the example of a methanation reactor in the context of power-to-gas applications, a dynamic optimization approach is used to identify control trajectories for time optimal reactor start-up which simultaneously inhibit distinct hot spot formation. Therefore, we develop a dynamic, two- dimensional model of a packed-bed tube reactor for carbon dioxide methanation which is based on the reaction scheme of the underlying exothermic Sabatier reaction mechanism [1]. However, dealing with large-scale nonlinear dynamical process models often leads to many computational difficulties. Facing this issue, snapshot-based model order reduction techniques, such as proper orthogonal decomposition together with the discrete empirical interpolation method (POD-DEIM) generate considerably less complex models, featuring a lower number of states and, furthermore, guarantee an acceptable model error [2]. Thus, these surrogate models show a significant potential for dynamic optimization tasks in terms of CPU time and memory costs [3]. We illustrate the applicability of POD-DEIM to the methanation rector and discuss the feasibility of integrating the obtained reduced-order models for dynamic optimization.

References

[1] Bremer, J., Rätze, K.H., and Sundmacher, K., CO₂ Methanation: Optimal Start-Up Control of a Fixed-Bed Reactor for Power-To-Gas Applications. AIChE Journal (2016).

[2] Benner, P., Gugercin, S., and Willcox, K., A Survey of Projection-Based Model Reduction Methods for Parametric Systems. SIAM Review (2015).

[3] Bremer, J., Goyal, P., Feng, L., Benner, P., and Sundmacher, K., *POD-DEIM for Efficient Reduction of a Dynamic 2D Catalytic Reactor Model.* Computers & Chemical Engineering (2016). *submitted*

Singularly perturbed vector fields, model reduction of reacting flow systems

Viatcheslav Bykov

Institute of Technical Thermodynamics, Karlsruhe Institute of Technology

The problem of dimensionality and complexity reduction of mathematical models of reacting flow systems is in the focus of the suggested talk. Geometrical methods e.g. regular and singular perturbations techniques, invariant manifolds method etc. will be discussed. The problem of model reduction is posed by using low-dimensional manifolds embedded in the reacting system state space. Thus, the problem is reduced to definition the lowdimensional manifolds, investigation their properties and construction of appropriate ones in the detailed thermo-chemical state space of a reacting system.

The suggested framework unifies three powerful methodologies to study dynamical systems: the methods of singular perturbations, the concept of invariant manifolds and the method of decomposition of motions. This makes developed approach very efficient in both analytical and numerical aspects. Analytical results will be presented and substantiated the use of fast and slow invariant manifolds in model reduction, while numerical implementations presented confirm its robustness and efficiency.

Interpolatory methods for H_{∞} model reduction of MIMO systems

Alessandro Castagnotto Technische Universität München

In this talk we present a computationally effective approach for producing high-quality H-infinity approximations to large-scale linear dynamical systems having multiple inputs and multiple outputs (MIMO). The proposed method extends the work by Flagg, Beattie, and Gugercin (2013), which combined ideas originating in interpolatory H2-optimal model reduction with complex Chebyshev approximation.

Our extension retains this framework and the original intuition behind the method. Starting from an H2-optimal reduced order model, we effectively reduce the H-infinity approximation error by performing constrained multivariate optimization, while preserving H2-optimal interpolatory conditions.

"Free" data-driven rational approximations, built upon previously computed function samples, are exploited to drastically reduce the computational burden of H-infinity norm evaluations, making this approach numerically efficient even for very large-scale models.

Numerical examples demonstrate the effectiveness of the proposed procedure, consistently showing better H-infinity performance than balanced truncation and at times even optimal Hankel norm approximation.

Model reduction of second-order electromechanical swing equations with structural preservation

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The model reduction of electromechanical swing equations is considered. The equations describes the networked power system which is modeled as a second-order system with matrix coefficients. The purpose is to derive a lower-dimensional approximation which still inherits a network structure. The proposed method is based on graph clustering, where the states with similar responses to the external inputs are placed into same clusters. Then, the reduced-order model is generated by the Petrov-Galerkin method, where the projection is formed by the characteristic matrix of the resulting network clustering. It is shown that the simplified system preserves an second-order structure as well as an interconnection topology. Thus, it can be again interpreted as a power system evolving over a reduced graph. Furthermore, we generalize the definition of network controllability Gramian, which leads to a convenient way to compute the approximation error.

Krylov subspace methods for model reduction of MIMO quadratic-bilinear systems

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Model order reduction for large-scale nonlinear dynamical systems has gained a lot of attention in the past ten years. Well-known simulation-based techniques like POD and TPWL are widely used, especially for the reduction of complex and strong nonlinear systems. Since these methods rely on expensive simulations for different training input signals, the reduced models are input dependent and might therefore yield moderate approximations when subjected to other excitation signals. In order to overcome this issue, popular linear system-theoretic reduction techniques like balanced truncation, Krylov subspace methods and H_2 optimal approaches have been recently generalized and successfully applied to bilinear [1, 5] and quadratic-bilinear systems [2, 3, 4].

In this talk, we focus on MIMO quadratic-bilinear systems. First, the systems theory and transfer function concepts known from the SISO case are studied and extended to the MIMO case. Then, new block and tangential Krylov reduction methods for MIMO quadratic-bilinear systems will be reported, analyzed and their performance compared.

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ISTEP as an example of nonlinear non-intrusive model order reduction technique

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Many systems like vehicle crashes, fluid-structure interactions or mechanical systems with large deformations cannot be considered as linear. Therefore, nonlinear model order reduction techniques are necessary. However, nonlinear model order reduction (MOR) techniques are much harder to implement - especially in combination with commercial solver and modeling packages. Nonlinear MOR needs to be implemented within commercial solvers, which is necessary to keep the users in their well-known simulation environment, but there is only minimal possibility to gain access to the solver and the underlying differential equations. In this work, the Stiffness Evaluation Procedure (STEP) is presented as a possibility to implement a very non-intrusive nonlinear MOR technique. The approximation strategy combining linear MOR with a Taylor approximation of the remaining nonlinear part is characterized by simplicity. We present here first results in terms of implementation friendliness with the nonlinear deformation of a car roof in Ls-Dyna.

SLIM-Decomposition of tensor train operators for nearest-neighbor interaction networks

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Low-rank tensor approximation approaches have become an important tool in the scientific computing community. The aim is to enable the simulation and analysis of highdimensional problems which cannot be solved using conventional methods anymore due to the so-called curse of dimensionality. We present a systematic tensor train decomposition for nearest neighbor interaction systems which is applicable to many different areas, e.g. quantum physics, chemical reaction dynamics and stochastic queuing problems. With the aid of this decomposition, it is possible to reduce the memory consumption as well as the computational costs significantly. Furthermore, it can be shown that in some cases the rank of the tensor decomposition does not depend on the network size and the format is thus feasible even for high-dimensional systems. The approach is illustrated using a first-principles based reduced model for the CO oxidation on the RuO₂ surface.

Online adaptive local-global POD-DEIM model reduction for fast simulation of flows in heterogeneous media

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Reduced order modeling techniques have been investigated in the context of reservoir simulation and optimization in order to mitigate the computational cost associated with the large-scale nature of the reservoir models. Although great progress has been made in basically three fronts, namely, upscaling, model reduction, and data driven modeling, there has not been a consensus which method (or methods) is preferable in terms of the trade-offs between accuracy and robustness, and if they indeed, result in large computational savings, especially in practical application of multiphase flow simulations. In this work, we will present advances these three fronts, and will show our recent work in localglobal model reductions techniques coupling multiscale finite element modeling (MsFEM) and POD-DEIM. To this end, we use local online error indicators to determine if global updates are necessary to control model accuracy. Local multiscale basis functions reduce the computational cost of the global update.

Balanced truncation for linear switched systems

Ion Victor Gosea^{*,1}, Athanasios C. Antoulas^{1,2} ¹Jacobs University Bremen, ²Rice University, Houston

We discuss a novel model order reduction approach towards balanced truncation of linear switched systems (LSS). Such systems switch among a finite number of linear subsystems or modes. We compute the controllability and observability gramians P and Qcorresponding to each active mode by solving generalized Sylvester equations. We show how these gramians provide lower and upper bounds for input and output energy functionals. In order to guarantee that hard to control and hard to observe states are truncated simultaneously, we construct a transformed LSS, whose gramians are equal and diagonal. Then, by truncation, we come up with reduced order models. We introduce a H_2 -type of norm both in time and in frequency domain and show how to effectively evaluate it. We illustrate the practical applicability of the proposed method by means of several numerical experiments such as a CD player example and a large scale mechanical example.

Interpolation-based optimal model reduction for a class of descriptor systems with application to Navier-Stokes equations

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We discuss model reduction for a special class of quadratic-bilinear (QB) descriptor systems which include semi-discretized Navier-Stokes equations. The goal is to extend the framework of truncated iterative Rational Krylov Algorithm (TQB-IRKA) for QB ODE systems [Benner et al. 16] to the aforementioned class of descriptor systems in an efficient and reliable way. Recent results have shown that direct application of interpolation-based model reduction techniques to linear descriptor systems, without any modifications, may lead to poor reduced-order systems. Therefore, for the analysis, we transform the QB descriptor system into an equivalent QB ODE system for which the TQB-IRKA is employed to obtain the reduced-order system. In view of implementation, we provide algorithms that identify the required Krylov subspaces without explicitly computing the projectors used in the analysis. The efficiency of the proposed modified TQB-IRKA for the class of descriptor systems is illustrated by means of the semi-discretized Navier-Stokes equations.

POD reduced order modeling for evolution equations utilizing arbitrary finite element discretizations

Carmen Gräßle^{*}, Michael Hinze University Hamburg

The main focus of the present work is the inclusion of spatial adaptivity for snapshot computation in the offline phase of model order reduction utilizing Proper Orthogonal Decomposition (POD-MOR). For each time level, the snapshots live in different finite element spaces, which means in a fully discrete setting that the snapshots are vectors of different length. In order to overcome this obstacle, we present a discretization independent POD reduced order model, which is motivated from a continuous perspective and is set up explicitly without interpolation of the snapshots. The analysis for the error between the resulting POD solution and the true solution is carried out. Finally, we present numerical examples to illustrate our approach.

Space-time Galerkin POD for optimal control of Burgers' equation

Manuel Baumann, Peter Benner, Jan Heiland *

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In the context of Galerkin discretizations of a PDE, the modes of the classical method of Proper Orthogonal Decomposition (POD) can be interpreted as the ansatz and trial functions of a low-dimensional Galerkin scheme. If one also considers a Galerkin method for the time integration, one can similarly define a POD reduction of the temporal component. This has been described earlier but not expanded upon – probably because the reduced time discretization globalizes time which is computationally inefficient. However, in finitetime optimal control systems, time is a global variable and there is no disadvantage from using a POD reduced Galerkin scheme in time. In this talk, we provide a newly developed generalized theory for space-time Galerkin POD, show its application for the control of the nonlinear Burgers' equation, and discuss the competitiveness by comparing to standard approaches like classical POD combined with gradient-based methods.

Towards empirical-Gramian-based model reduction for nonlinear DAEs

Peter Benner, Sara Grundel, Christian Himpe^{*} Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg

The simulation of energy systems requires evaluations of nonlinear PDEs subject to conservation principles. Specifically gas transport in a network of pipelines can be modeled by the Euler equation including mass conservation and pressure balance. Spatially discretized, a gas network is then described by a system of nonlinear DAEs, which by a selection of relevant quantities of interest becomes an input-output system. To accelerate the repeated simulation of such a network in a transient phase, subsequent to a perturbation of a steady supply and demand condition, a data- driven model reduction method, based on empirical Gramian matrices, is tested. We present a comparison of empirical-Gramianbased model reduction techniques applied to different variants of a gas network model, assess the difficulties of these methods for nonlinear DAE models and propose extensions to the empirical Gramian approach to improve the accuracy of the reduced-order models.

Parametrized Sylvester equations in model order reduction

Manuela Hund^{*}, Jens Saak

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Sylvester equations of the form

$$AV\tilde{E} + EV\tilde{A} = BL \tag{1}$$

are a key player in model order reduction (MOR) of linear input-output systems as

$$E\dot{x}(t) = Ax(t) + Bu(t),$$

$$y(t) = Cx(t),$$

with a regular matrix $E \in \mathbb{R}^{n \times n}$, as well as matrices $A \in \mathbb{R}^{n \times n}$, $B \in \mathbb{R}^{n \times p}$, $C \in \mathbb{R}^{q \times n}$ and $\tilde{A}, \tilde{E} \in \mathbb{R}^{m \times m}$, where $m \ll n$.

These arise in the context of the \mathcal{H}_2 optimality conditions of Wilson, the variation of the orthogonal polynomial time domain MOR framework of Jiang and Chen, as well as in classical moment matching.

There are different ways parametrized Sylvester equations may arise in MOR. On the one hand, in the time domain approach, one ends up with a Sylvester equation (1), where \tilde{A} is the identity $I_m \in \mathbb{R}^{m \times m}$. The solution of this Sylvester equation is equal to the Krylov subspace using moment matching with the generalized eigenvalues of (I_m, \tilde{E}) as expansion points. Now, when using parametrized families of Jacobi polynomials, a Sylvester equation

$$AVE(a,b) + EV = BL,$$

arises, that is parametrized in the small matrix E(a, b).

On the other hand, considering parametrized dynamical systems

$$E(t,\mu)\dot{x}(t) = A(t,\mu)x(t) + B(t,\mu)u(t),$$

$$y(t) = C(t,\mu)x(t),$$
(2)

with parameter $\mu \in \mathbb{R}^d$, provides a Sylvester equation that is now parametrized in its large, but sparse matrices

$$A(t,\mu)V\tilde{E} + E(t,\mu)V\tilde{A} = B(t,\mu)L.$$

Our final goal is to solve the \mathcal{H}_2 optimal MOR problem via a fixed point iteration on the Wilson conditions along the lines of the two sided iterative approximation (TSIA) algorithm. This could in turn serve as an alternative parametrized \mathcal{H}_2 optimal MOR algorithm to the "parametric IRKA". In our contribution, we will present first results towards this goal.

Automatic model reduction of differential algebraic systems by proper orthogonal decomposition

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Proper Orthogonal Decomposition is a technique for obtaining reduced models of low order. The automatization of the mentioned reduction method is presented, which is implemented as a stand-alone software tool. The tool provides an environment that performs the model reduction of differential algebraic systems automatically with minimal additional input from the user. The Empirical Interpolation method is used for approximation of the system's nonlinearity. The software tool has been applied to a nonlinear heat conduction model and a continuous fluidized bed crystallizer model. The automatically generated reduced models are significantly smaller than the reference models. An a-posteriori error estimator is used to assess the quality of the reduced models during runtime. Since the estimation efficiency is of great importance, the used error estimator assesses the system's output error rather than the error of the state vector, as for many applications the output is much more important than the internal states.

Dynamic mode decomposition and extensions

Stefan Klus Freie Universität Berlin

Over the last years, numerical methods to analyze large data sets have gained a lot of attention. Recently, different purely data-driven methods have been proposed which enable the user to extract relevant information about the global behavior of the underlying dynamical system, to identify low-order dynamics, and to compute finite-dimensional approximations of transfer operators associated with the system. However, due to the curse of dimensionality, analyzing high-dimensional systems is often infeasible using conventional methods since the amount of memory required to compute and store the results grows exponentially with the size of the system. This can be mitigated by exploiting low-rank tensor approximation approaches. The goal of this talk is twofold: First, we will present data-driven methods for the analysis of complex dynamical systems such as Dynamic Mode Decomposition (DMD) and Extended Dynamic Mode Decomposition (EDMD). Secondly, we will show how these methods can be reformulated in terms of tensors.

Reduced basis method for Poisson-Boltzmann equation

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The Poisson-Boltzmann equation (PBE) is an elliptic PDE that arises in biomolecular modeling to determine the electrostatic potential around a biomolecule in an ionic solution. Solving the PBE numerically is computationally quite challenging due to the long range nature of electrostatic interactions and also due to the need to solve the PBE at many values of physical parameters, such as the ionic strength. In this study, we discretize the linearized PBE with a centered finite difference scheme and the resulting parametrized linear system is solved by the preconditioned conjugate gradient (PCG) method. Reduced basis method (RBM) is applied to the high-fidelity full order model (FOM) and the discrete empirical interpolation method (DEIM) is employed to reduce the complexity of the online phase of the RBM due to the nonaffine parameter dependence of the Dirichlet boundary conditions. From the numerical results we notice that the RBM reduces the order of the FOM from 2 million to 6 at a high accuracy and reduces computational time by a factor of 7600. On the other hand, DEIM provides a speed-up of 20 at a single iteration of the greedy algorithm in the online phase.

Time- and frequency-limited balanced truncation for large-scale systems

Patrick Kürschner

Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg

The well established balanced truncation model order reduction methodology can be modified to a form, where the reduced order models only need to be accurate in restricted time- or frequency intervals. Compared to ordinary balanced truncation without such restrictions, these time- and frequency-limited versions come with additional difficulties from a numerical point of view, especially for large-scale systems. We present recent results regarding a new efficient numerical realization of time- and frequency-limited balanced truncation, making it actually executable in the large-scale case. With this approach, timeand frequency-limited balanced truncation can outperform unrestricted balanced truncation w.r.t. both accuracy and computational costs. If time permits, some perspectives for the reduction of unstable systems are given.

Application of a tensor product decomposition method to turbulent data

Thomas von Larcher^{1,*}, Rupert Klein¹, Reinhold Schneider², Sebastian Wolf², Benjamin Huber²

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Low-rank multilevel approximation methods are an important tool in numerical analysis and in scientific computing. Those methods are often suited to attack high-dimensional problems successfully and allow very compact representations of large data sets. Specifically, hierarchical tensor product decomposition methods emerge as an promising approach for application to data that are concerned with cascade-of-scales problems as, e.g., in turbulent fluid dynamics. We focus on two particular objectives, that is representing turbulent data in an appropriate compact form and, secondly and as a long-term goal, finding selfsimilar vortex structures in multiscale problems. The question here is whether the new tensor product methods can support the development of improved understanding of the multiscale behavior and whether they are an improved starting point in the development of compact storage schemes for solutions of such problems relative to linear ansatz spaces. We present the reconstruction capabilities of a tensor decomposition based modeling approach tested against 3D turbulent channel flow data.

On structure preserving model order reduction for damped wave propagation on networks

Björn Liljegren-Sailer^{1,*}, Herbert Egger², Thomas Kugler², Nicole Marheineke¹ ¹Friedrich-Alexander-Universität Erlangen-Nürnberg, ²TU Darmstadt

We consider a partial differential algebraic system describing the propagation of pressure waves in a pipeline network and aim for an efficient simulation with the help of model order reduction tools. The system inherits important physical properties as mass-conservation, passivity, existence of unique steady states and exponential stability. Appropriate space discretizations, which inherits the upper properties, can be constructed e.g. by mixed finite element methods. We seek for low-order reduced models constructed from these space discretizations by a projection ansatz, which also guarantee the relevant physical properties. For this purpose a detailed analysis in a function space setup is needed, as well as an algebraic characterization of the needed compatibility conditions. Numerical results using Pade-type approximations will be shown, which also demonstrate the necessity of the compatibility conditions.

Interpolation strategy for parametric QBMOR for gas pipeline-networks

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Optimization and control of large transient gas networks require the fast simulation of the underlying parametric partial differential algebraic systems. In this talk we present a surrogate modeling technique that is composed of quadratic bilinearizaton (QB), spatial semi-discretization and model order reduction (MOR) via moment-matching. Nonzero initial values may lead to worse error-behavior for MOR. We show an improvement and discuss about its advantage and drawback. Additionally, we show that QB-pROMs can be evaluated over a wide parameter range of different boundary pressures and temperatures by using the matrix interpolation.

Model reduction of network systems by clustering

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We present an efficient clustering-based model order reduction method for linear, diffusively coupled, multi-agent systems. The method combines an established model order reduction method and a clustering algorithm to produce a graph partition used for reduction, thus preserving the network structure and consensus. By the Iterative Rational Krylov Algorithm, a good reduced order model can be found which is not necessarily structure preserving. However, based on this we can efficiently find a partition using the QR decomposition with column pivoting as a clustering algorithm, so that the structure can be restored. To demonstrate the flexibility of this approach, we combine a nonlinear model order reduction method and a clustering algorithm to reduce nonlinear multi-agent systems by clustering. We illustrate the effectiveness of the method on a number of examples.

A-priori element selection and weighting for hyper-reduction in nonlinear structural dynamics

Frank Naets

K.U. Leuven - Mechanical Engineering Division PMA (Production Engineering, Machine Design and Automation)

The energy-conserving sampling and weighting (ECSW) was recently proposed as a stability preserving scheme for nonlinear (structural) finite element model reduction. However, this scheme requires (several) reference simulation(s) to be performed in order to train the reduced order model (ROM). The cost of this training on the high-fidelity model can be unacceptable in many applications.

This work proposes a new sampling approach for the element selection in the ECSW framework which can be exploited for a-priori element selection. In this approach a non-negative L1 optimization is performed which selects the element to match the reduced stiffness and internal forces for a given reference configuration of the model. This element selection can be used both with an a-priori constructed modal (derivative) basis and with an a-posterior constructed POD basis. Numerical validation on several examples demonstrate the speed and accuracy of this approach.

Variational tensor approach to the rare-event kinetics of macromolecular systems

Feliks Nüske

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In this talk, I will present an application of tensor product approximations to molecular dynamics (MD) simulations. A major goal in biochemistry is the determination of long lived geometrical structures (metastable conformations) of a molecule. These can be detected using the dominant spectral components of the transfer operator of the Markov process sampled by MD. A variational formulation allows to approximate the eigenfunctions from a finite-dimensional trial space. We have suggested to use a basis set comprised of tensor products of physically meaningful functions, describing, for instance, the formation / breaking of a contact. In order to deal with the explosion of basis set size, we have used the tensor train format and the related learning algorithm ALS to compute a suitable lowrank approximation. I will show two benchmark applications and, if time allows, discuss a combination with observable operator models (OOMs) and short simulations to analyze large systems.

Reduced basis methods for the design of stabilizing feedback controllers

Robert O'Connor^{*}, Martin Grepl RWTH Aachen University

Many real-world systems are described by PDEs that need to be discretized if we wish to simulate the systems. Unfortunately, traditional discretization methods produce very high-dimensional models, which are often unpractical and need to be simplified. One way to simplify such models is the reduced basis method. It allows us to efficiently approximate solutions for a large number of parameter values. Existing reduced basis methods build models that attempt to minimizes the error in a given norm. For simulations, optimization, and even optimal control such methods work quite well. Feedback, however, is fundamentally different: Unlike optimal control, it changes the system's dynamics. As a result, ensuring the stability of the closed-loop system is an essential part of designing a feedback controller. We present a novel reduced basis method to handle the distinct challenges of stabilizing feedback control.

Parametrized model order reduction for second order systems with a low rank change in the system matrices

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Recently, a parametric model order reduction scheme was developed that allows for low rank variability in the state matrices, but does not require an a priori sampling of the parameter space. In this work the methodology is extended to second order dynamic systems, allowing for an independent low rank variability in both the stiffness and damping matrix. This is achieved by augmenting the input and output vectors and shifting the parameter dependence to the throughput matrix of the state space model. A second order Arnoldi scheme is used to obtain the projection matrix required for calculating the reduced order model. The effectiveness of the method is shown by applying it on a finite element model of a plate, in which the aim is to find the precise location and severity of a crack. The potential crack locations are parametrized by a local stiffness variation.

Decay of singular values for infinite-dimensional control systems

Mark Opmeer

Department of Mathematical Sciences, University of Bath

We show that the observability Gramian of an (infinite-dimensional) linear control system with an analytic semigroup, an observation operator which is not too unbounded and with a finite-dimensional output space, has singular values which decay exponentially in the square root.

As a corollary it is shown that the Hankel singular values of such a control system (with an input operator which is not too unbounded and with possibly an infinite-dimensional input space) also decay exponentially in the square root. Another corollary shows that the solutions of various algebraic Riccati equations for such systems also have singular values with the same decay rate. The considered Riccati equations include the standard LQR control Riccati equation, but also the Strictly Bounded Real and Positive Real Riccati equations.

These results are based on the trapezoidal rule for approximating integrals of Banach space valued analytic functions.

Replicability, Reproducibility and Reusability for Model Order Reduction (RRR 4 MOR)

Jens Saak

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There is no advanced computer-based simulation of complex systems without model order reduction (MOR) and there is no MOR without scientific computing.

Typically, new or improved MOR techniques are not only mathematically proven to be applicable, but often also confirmed numerically. Even more, if a theoretical proof is not obtained, numerically a method's viability can still be demonstrated. In either case, computer-based experiments (CBEx) are an essential component of MOR research. To enhance and ensure scientific standards for these CBEx we propose a set of general best practices, which aim at replicability of one's own research, enable reproducibility for others, and accelerate improvements through reusability. The presented guidelines are simple, language-agnostic and illustrated by examples.

Symmetry reduction without equivariance in reduced order models

Matthew Salewski

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Transport-dominated dynamical systems continue to withstand current methods of model reduction and require new strategies. One such approach is symmetry reduction, also known as the method of freezing, where the effect of continuous-parameter transformation groups is reduced from the solution space resulting in dynamics where the transport is diminished or removed. In fact, solutions which support transport phenomena are often found in systems which admit translation invariance; symmetry reduction works by removing this degree of freedom. We demonstrate reduced basis models, including hyper-reduction, built using symmetry reduction for some standard systems with transport phenomena. A usual prerequisite for symmetry reduction is the equivariance of the vector field of the dynamical system with respect to the action of a continuous parameter transformation. We show that this condition is flexible, which can lead to systems that are more amenable to model reduction.

An adaptive sampling strategy for MIMO surrogate models based on merging (Co-)kriging and POD

Anna Sauerbrei^{1,*}, Ralf Zimmermann²

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In many practical applications numerical models with multiple inputs and multiple outputs play an important role. But high-fidelity models are often computationally expensive and therefore unfeasible for the use in optimization processes. Therefore, surrogate models are used to improve the efficiency of such optimization processes. One known approach to construct surrogate models is to combine the statistical interpolation method Co-Kriging with the proper orthogonal decomposition (POD). The method is non-intrusive in the sense that the underlying high-fidelity model acts as a black box function and no intrinsic modifications are required. During this talk, a new adaptive sampling strategy is introduced to effectively improve the accuracy of the surrogate model until a desired level is reached.

Damping optimization of parameter dependent mechanical systems by rational interpolation

Zoran Tomljanovic^{1,*}, Christopher Beattie², Serkan Gugercin² ¹Department of Mathematics, Josip Juraj Strossmayer University of Osijek ²Department of Mathematics, Virginia Tech

We consider the problem of optimization of semi-active damping of vibrating systems. The main problem is to determine the best damping matrix which will minimize the influence of the input to the output. We use a minimization criteria based on the H_2 system norm. Since that the objective function is a non-convex function, this damping optimization problem usually requires a large number evaluations of objective function. Thus, we propose an optimization approach that calculates the interpolatory reduced model which allows significant acceleration of optimization.

In our approach we use parametric model reduction based on Iterative Rational Krylov Algorithm, which ensures a good approximation of objective function. The sampling parameters for the parametric model reduction can be calculated using fixed or adaptive sampling parameters.

This approach provides a significant acceleration of the optimization process, which will be illustrated in numerical experiments.

Hankel-norm approximation of descriptor systems

Steffen Werner^{*}, Peter Benner

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The main aim of model reduction is always to approximate the original system by a reduced one. Beside this, a measure for the approximation error in a certain system norm is desired. The system norm which measures the amount of influence of the past inputs u_{-} on future outputs y_{+} in the \mathcal{L}_{2} sense is the Hankel-norm

$$||G||_{H} = \sup_{u_{-} \in \mathcal{L}_{2}} \frac{||y_{+}||_{\mathcal{L}_{2}}}{||u_{-}||_{\mathcal{L}_{2}}}.$$

Considering the case of linear time-invariant continuous-time standard systems,

$$\dot{x}(t) = Ax(t) + Bu(t),$$

$$y(t) = Cx(t) + Du(t),$$

the Hankel-norm is simply given by the largest Hankel singular value of the system. Also it is possible for the standard case to construct a reduced-order best approximation in the Hankel-norm. A well known model reduction method for this purpose was introduced by Glover (1984).

But the modeling of many applications, like mechanical systems and computational fluid dynamics, result in descriptor systems

$$\begin{aligned} E\dot{x}(t) &= Ax(t) + Bu(t), \\ y(t) &= Cx(t) + Du(t), \end{aligned} \tag{3}$$

with a singular E matrix. For the reduction of such systems a generalized version of the Hankel-norm approximation method is needed. One approach based on the Weierstrass canonical form is given by Cao, Saltik, and Weiland (2015). The problem here is the numerically unstable computation of the Weierstrass canonical form.

A much more efficient approach for general linear descriptor systems can be derived from the generalized balanced truncation method, see Mehrmann, Stykel (2005).

Parametric model order reduction for efficient uncertainty quantification in the electro-thermal analysis of nanoelectronic devices

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In robust design of nanoelectronic devices, both electro-thermal analysis and uncertainty quantification are indispensable. However, an accurate electro-thermal model in the state-space, which is often used in computational analysis, is usually of a large dimension. This poses a computational challenge to uncertainty quantification: e.g., a non-intrusive method requires repeatedly simulating the large-scale system at various parameter values. Therefore, parametric model order reduction, which efficiently builds a small-scale model valid on a specified parameter range, serves as a powerful tool for acceleration. To obtain a compact reduced-order model, we develop a specific method to reduce one-way coupled parametric models arising from electro-thermal analysis of nanoelectronic devices. The resulting reduced-order model is used as a surrogate in two non-intrusive methods for uncertainty quantification: Latin hypercube sampling and stochastic collocation. Numerical results for a Power-MOS device validate the accuracy and efficiency of the proposed uncertainty quantification methods based on parametric model order reduction.

A novel POD-based model order reduction at the substructure level for nonlinear structural analysis

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For a nonlinear finite element-based structural analysis, a novel model reduction method at the substructure level is proposed. The finite element analysis of a complex modular structure which consists of regular substructures, involves a large number of degrees-of-freedom leading to high computational effort. In order to reduce the number of degrees-of-freedom of the substructures individually and thereby the dimension of the global equation system, model order reduction is applied on the substructures. In the proposed method, the projection-based reduction is applied on each substructure, with their complete modes including internal and boundary nodes. For the coupling, a new surface-to-surface contact formulation using the penalty method is presented, which couples the reduced and unreduced substructures consisting of nonmatching meshes. Several numerical examples have been investigated. They show the good performance of the method as well as the convergence behaviour in the coupling and reduction process.

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